

Scaling property of the critical hopping parameters for the Bose-Hubbard model

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Abstract. Recently precise results for the boundary between the Mott insulator phase and the superfluid phase of the homogeneous Bose-Hubbard model have become available for arbitrary integer filling factor g and any lattice dimension $d \geq 2$. We use these data for demonstrating that the critical hopping parameters obey a scaling relationship which allows one to map results for different g onto each other. Unexpectedly, the mean-field result captures the dependence of the exact critical parameters on the filling factor almost fully. We also present an approximation formula which describes the critical parameters for $d \geq 2$ and any g with high accuracy.

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In the last ten years experiments with ultracold atoms in optical lattice potentials generated by laser beams have become an important tool for mimicking phenomena in solid state physics, and have contributed to further understanding of many-particle systems [1,2]. Outstanding examples are the observation of Bloch oscillations [3,4], the direct measurement of Anderson localisation [5], or the detection of the Mott insulator-to-superfluid transition [6]. A model of utmost importance in this field of research is the Bose-Hubbard model. It describes a system of interacting ultracold bosons in an optical lattice [7], and has been intensively studied since the late eighties with numerous methods (see *e.g.* [1,2] and references therein). Nevertheless, the Bose-Hubbard model still is a topic of active research [8,9,10,12,11].

Although many techniques have been developed in order to calculate the phase diagram of the homogeneous Bose-Hubbard model, the evolution of the phase boundary between the Mott insulator and the superfluid phase with increasing filling factor so far has not been investigated thoroughly. For example, filling factors greater than one typically occur in experiments with a superimposed harmonic trap, which is necessary for confinement reasons. Then a wedding cake structure emerges with decreasing filling from the trap centre to the outer region. High-order perturbation theory utilising a process-chain approach [13] has made the regime of larger filling accessible only very recently, and has provided accurate data of the critical parameters for arbitrary integer filling factors.

In this communication we report a general scaling property of the critical hopping parameters with increasing filling factor. This scaling renders the critical parameters (almost) independent of the filling. Moreover, we present an approximation formula for the critical hopping for any dimension $d \geq 2$, and any filling factor. We proceed as follows: First the Bose-Hubbard model is briefly recapitulated. We then compare the phase boundary obtained via the process-chain approach [14] for unit filling ($g = 1$) with two recent high-precision results [8,11]. The excellent agreement serves to underline the high accuracy of the process-chain approach, which also provides data for higher filling factors, for which no reference data are available. After that, we apply three successively more accurate scalings to the critical parameters belonging to different filling factors. Finally, we develop the approximation formula, and end the letter with some concluding remarks.

1 The Bose-Hubbard model

Ultracold bosons in an optical lattice are fairly well described by the Bose-Hubbard model as long as the lattice is sufficiently deep [7]. In the limit of zero temperature only the lowest Wannier state at each individual site has to be considered, leading to a single-band model. Furthermore the on-site approximation is applied, *i.e.* it is assumed that only particles sitting on the same lattice site interact with each other. This interatomic repulsion leads to an increase of energy by U for each pair of interacting particles. Restricting the hopping processes to adjacent sites only, and denoting the matrix element connecting

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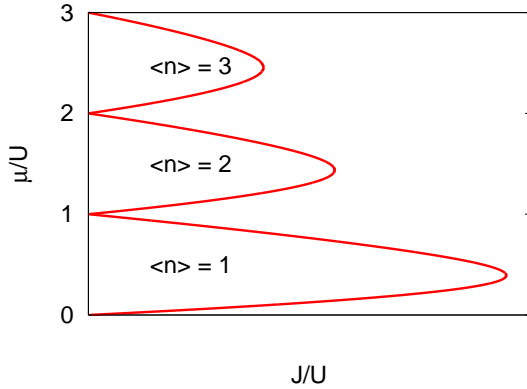


Fig. 1. Phase diagram of the Bose-Hubbard model, showing the three lowest Mott lobes. Inside the lobes the occupation number $\langle \hat{n} \rangle$ is fixed.

two neighbouring sites by J , one arrives at the well-known Bose-Hubbard Hamiltonian (see *e.g.* [7]):

$$H = -J \sum_{\langle i,j \rangle} \hat{a}_i^\dagger \hat{a}_j + \frac{U}{2} \sum_i \hat{n}_i (\hat{n}_i - 1) - \mu \sum_i \hat{n}_i. \quad (1)$$

The operators \hat{a}_i^\dagger and \hat{a}_i are the bosonic creation and annihilation operators for site i , and $\hat{n}_i = \hat{a}_i^\dagger \hat{a}_i$ is the corresponding number operator. The subscript $\langle i, j \rangle$ indicates that the sum is restricted to nearest neighbours. As we intend to describe a homogeneous system, the chemical potential μ is constant. The competition between the kinetic energy, described by the first term of the Hamiltonian (1), and the interaction energy (second term) gives rise to a quantum phase transition from a Mott-insulating to a superfluid phase upon increasing the hopping strength [15].

When using the pair interaction energy U as the energy scale of reference (*i.e.* when dividing eq. (1) by U) the Hamiltonian is governed by two dimensionless parameters: The hopping parameter J/U and the scaled chemical potential μ/U . In case of $J/U \ll 1$ the system is in a Mott phase, in which particles tend to localise at the individual sites. A fixed number of atoms occupies each lattice site and thus the system is incompressible: $\partial \langle n_i \rangle / \partial \mu = 0$. On the other hand, when $J/U \gg 1$, the particles tend to delocalise, and phase fluctuations are suppressed. The bosons then condense into the lowest Bloch state and the system is superfluid. Figure 1 sketches the phase diagram in the J/U - μ/U -plane. Inside the Mott lobes the occupation number $\langle \hat{n} \rangle$ is integer, while outside the lobes – in the superfluid phase – it can take on any rational value. The lobe's width at a fixed tunneling rate corresponds to the energy gap for a particle-hole excitation, which represents an important experimentally accessible quantity. It vanishes when the hopping strength exceeds the critical value $(J/U)_c$. For integer μ/U and $J/U = 0$ the system's ground state is highly degenerate, as either μ/U or $\mu/U + 1$ particles can occupy each site. Qualitatively the phase diagram has already been understood by Fisher *et al.* [16].

The mean-field phase boundary, given by

$$(J/U)_{\text{pb}} = \frac{1}{2d} \frac{(\mu/U - g + 1)(g - \mu/U)}{\mu/U + 1}, \quad (2)$$

was derived within a model which embodies equal couplings between all sites. Here d is the dimensionality of the lattice and g is the integer number of particles per site, referred to as the filling factor of the optical lattice. Precise quantitative results for the phase boundary of the three-dimensional homogeneous Bose-Hubbard model have been obtained by Quantum Monte Carlo simulations [8], and by means of a strong coupling expansion together with a scaling analysis [11], for $g = 1$. So far, a precise analysis of the behaviour of the phase boundary with increasing filling factor has not been performed. It should be pointed out that accurate data for the phase boundary are hard to obtain at higher fillings, as the dimensionality of the Hilbert space rapidly grows with increasing number of particles.

2 Comparison of approaches for unit filling

Recently dos Santos *et al.* derived the phase boundary for the Bose-Hubbard model by applying the method of the effective potential [10]. Employing the process-chain approach [13] together with the effective potential method, high orders in the hopping parameter J/U have become accessible, resulting in precise phase boundaries for dimensions $d \geq 2$ and arbitrary integer filling factors [14]. Figure 2 displays a comparison between the boundaries for $g = 1$ obtained within three different methods: the process-chain approach (PCA), a strong coupling expansion paired with a scaling analysis [11], and Quantum Monte Carlo simulations [8]. The latter two techniques are known to be highly accurate, so that the perfect agreement proves the reliability of the PCA data for unit filling. In the following we rely on the fact that the process-chain approach reaches comparable accuracy for any g .

3 Scaling behaviour with increasing filling

In order to monitor the evolution of the phase boundary with increasing filling factor g we concentrate on the critical value $(J/U)_c$, which is defined by the maximum hopping parameter of the respective Mott lobe. All outcomes reported here are obtained by a high-order perturbation calculation up to eighth order in J/U , with an additional extrapolation to infinite order. For a detailed explanation how to apply the process-chain approach to the Bose-Hubbard model we refer to ref. [17]. Although the data employed here were calculated for a hypercubic lattice, one can apply the same technique to other types of lattices such as triangular ones or ladder systems.

The usual expectation that $(J/U)_c$ scales like $\sim 1/g$ for high fillings g is borne out by the upper plot in fig. 3, since the scaled critical hopping

$$\left(\frac{J}{U} \right)_c = g \left(\frac{J}{U} \right)_c, \quad (3)$$

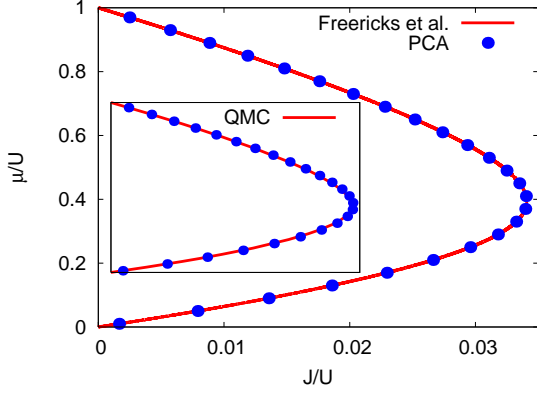


Fig. 2. Comparison of phase boundaries for $d = 3$ and unit filling ($g = 1$) obtained from the process-chain approach (PCA, ref. [14]), and from the scaling approach (Freericks *et al.*, ref. [11]). The inset includes data from Quantum Monte Carlo simulations (QMC, ref. [8]). Especially the results by Freericks *et al.* are virtually indistinguishable from our findings, while the QMC data show exiguous deviations close to the tip [17].

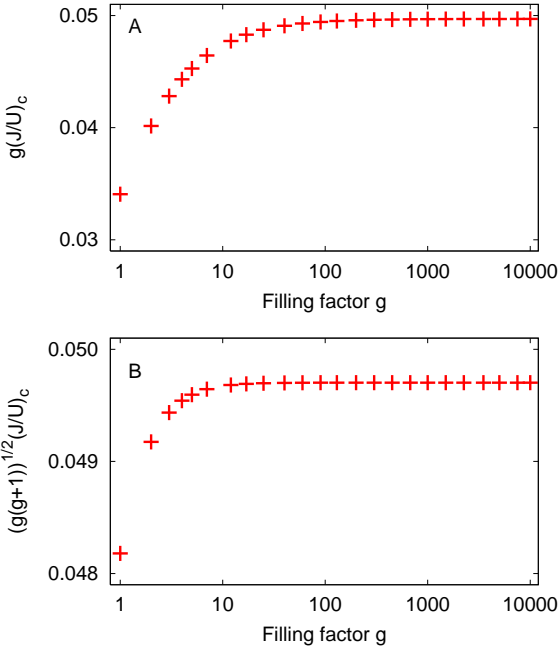


Fig. 3. Critical hopping parameters $(J/U)_c$ for various filling factors g in three dimensions and two different kinds of scaling. A: The values are scaled by the factor g . B: The values are scaled by the factor $\sqrt{g(g+1)}$. Note the finer scale in the lower figure.

approaches a constant for large g . But these scaled hopping parameters still cover a broad range (from 0.034 to 0.05), amounting to a variation of 32% and thus indicating that this type of scaling might be suboptimal. Indeed, a considerably better picture is obtained when employing

the phenomenological scaling

$$\left(\frac{\widetilde{J}}{U}\right)_c = \sqrt{g(g+1)} \left(\frac{J}{U}\right)_c, \quad (4)$$

which was discovered in ref. [17] for energy corrections, and which stems from the factors gained by successive hopping processes on a lattice with g particles per site on average. As the lower plot in fig. 3 shows, the improvement over the simple ansatz (3) displayed in the upper plot of fig. 3 corresponds to a factor of 10: The scaled critical parameters now range only from 0.048 to 0.050, amounting to a variation of 3.1%. Of course, in the limit of high filling factors both scalings yield the same results, as then $\sqrt{g(g+1)} \approx g$.

Although eq. (4) already leads to satisfying results, a further improvement can be achieved by examining the mean-field phase boundary of the Bose-Hubbard model, which is exact in the limiting case of infinite dimensionality (see *e.g.* [14]). By finding the maxima of eq. (2) with respect to the scaled chemical potential μ/U , the critical mean-field hopping parameters are identified as

$$\left(\frac{J}{U}\right)_c^{\text{MF}} = \frac{1}{2d} \left(2g + 1 - 2\sqrt{g(g+1)}\right). \quad (5)$$

Under the hypothesis that this dependence on the filling factor g also describes the g -dependence for finite dimensionality, we attempt the scaling

$$\left(\frac{\widetilde{J}}{U}\right)_c = \frac{1}{4} \left(2g + 1 - 2\sqrt{g(g+1)}\right)^{-1} \left(\frac{J}{U}\right)_c, \quad (6)$$

where the factor of $1/4$ has been included in order to ensure that the entire prefactor correctly reduces to g for high filling. As witnessed by fig. 4 for $d = 3$, this scaling works astonishingly well: The scaled parameters depicted there vary by merely 0.12%. In view of the accuracy of the process-chain approach itself, which is about 1% for $(J/U)_c$ in a three-dimensional system [14], these scaled critical parameters (6) can be regarded as constant. For other dimensions d we find the same marvellous mapping, making the critical hopping strengths practically independent of the filling factor g .

One can rewrite the ansatz (6) and finds after some lines of algebra

$$\left(\frac{\widetilde{J}}{U}\right)_c = \sqrt{g(g+1)} \left[\frac{1}{2} + \sqrt{\frac{1}{4} + \frac{1}{16g(g+1)}} \right] \left(\frac{J}{U}\right)_c, \quad (7)$$

which reveals that this scaling covers the two previous attempts of eqs. (3) and (4) in the limit of high filling factors g . Hence we conclude that for any d the functional dependence on the filling factor is correctly reflected by the scaling (7), which was extracted from the mean-field result (5). This appears to be unexpected, and could not be validated before reliable data for large g have been available. Of course, deviations of $(J/U)_c$ itself from the mean-field result due to finite dimensionality remain.

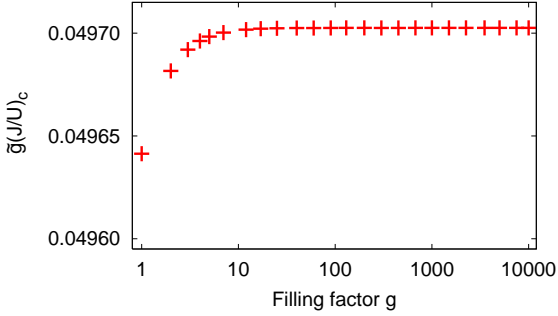


Fig. 4. Critical hopping parameters $(J/U)_c$ for various filling factors g in three dimensions. The values are scaled by the factor $\tilde{g} = \sqrt{g(g+1)} \left(\frac{1}{2} + \sqrt{\frac{1}{4} + \frac{1}{16g(g+1)}} \right)$, which emerges in the mean-field limit. Observe the fairly fine scale.

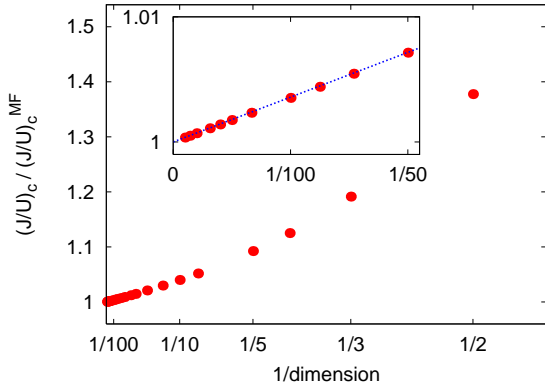


Fig. 5. Critical hopping parameter $(J/U)_c$ normalised by the mean-field value $(J/U)_c^{\text{MF}}$ plotted versus $1/d$ for unit filling. The inset shows a magnification for high d and includes a linear fit $f(1/d) = 1 + 0.358/d$ indicated by the dotted line.

4 An approximation formula for the critical hopping

With the process-chain approach one is also able to monitor the convergence of the critical hopping parameter towards the mean-field prediction (5) with increasing lattice dimensionality d . When plotting the relative values $(J/U)_c / (J/U)_c^{\text{MF}}$ of the critical parameters versus $1/d$, this convergence can be nicely watched. Figure 5 shows that even for quite high dimensionalities d of the lattice the mean-field theory substantially overestimates the critical hopping, for instance, by 4% for $d = 10$. The deviations in two and three dimensions are as large as 38% and 19%, respectively.

In order to set up an approximation formula for the critical hopping parameter for every dimension and arbitrary filling factor, one can now focus on the dimension-dependence since the dependence on the filling factor g is already accurately described by the scaling (7). We therefore perform our investigations on the data for unit filling. A reasonable ansatz for $(J/U)_c(d, g)$ is an expansion in

$1/d$:

$$\left(\frac{J}{U} \right)_c(d, g) = \left(\frac{J}{U} \right)_c^{\text{MF}} \left[1 + \sum_{\ell=1}^N a_{\ell} \frac{1}{d^{\ell}} \right]. \quad (8)$$

Indeed we find a mainly linear dependence on $1/d$ for high dimensions d , as shown by the inset of fig. 5. Fixing $N = 3$, fitting the expansion (8) to the data points given in fig. 5, and inserting $(J/U)_c^{\text{MF}}$, one obtains

$$\begin{aligned} \left(\frac{J}{U} \right)_c(d, g) &= \frac{1}{2d} (2g + 1 - 2\sqrt{g(g+1)}) \\ &\times \left[1 + 0.35 \frac{1}{d} + 0.39 \frac{1}{d^2} + 0.84 \frac{1}{d^3} \right]. \end{aligned} \quad (9)$$

This formula approximates the critical values $(J/U)_c$ obtained within the framework of the process-chain approach with an accuracy of better than 0.15%. Up to first order in $1/d$ findings deducible from ref. [10] are in very good agreement with this result.

5 Conclusion

When employing the method of the effective potential combined with the process-chain approach, one obtains high-precision data for the critical hopping parameter $(J/U)_c$ for any lattice dimension $d \geq 2$ and arbitrary integer filling factor g . These values show excellent agreement with other recent findings for the case $d = 3$ and $g = 1$ [8,11], thus gauging the accuracy of the data. We have shown that the relatively simple scaling (7), which was taken over from the mean-field result, maps the data for different filling factors almost perfectly onto each other. Hence the dependence of $(J/U)_c$ on the filling g is known with high precision. Although not theoretically deduced but accurately fitted, we have presented an excellent approximation formula [eq. (9)], which provides $(J/U)_c$ for any dimensionality $d \geq 2$ and any filling factor g for the homogeneous Bose-Hubbard model. These results may serve as benchmarks for future developments of other methods.

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